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On the applicability of the approximated Thomas-Fermi potentials in the low and intermediate energy regions

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Thomas-Fermi type ion-atom potentials, approximated by Lindhard for low and intermediate energy regions, have been used in evaluating computationally the binary collision scattering angle for argon ion with gold and silver atoms by solving the classical equations of motion. Assuming a logarithmic relation between the impact parameter for $\pi/2$ scattering and incident ion energy, the applicability of the forms of potential for a particular range of energy is discussed in the light of the available experimental results.

1. INTRODUCTION

Lindhard (1965) used the Thomas-Fermi ion-atom potential in his theory of channeling which was of the form

$$V(R) = (z_1 z_2 e^2/R)\phi_0(R/a),$$

where the subscripts 1 and 2 refer to the projectile and target atoms respectively. The screening parameter a is given by

$$a = 0\cdot8853 a_0/(z_1^{2/3}+z_2^{2/3})^{\frac{1}{2}}$$

where a_0 is the Bohr radius.

He obtained the string potential by averaging this $V(R)$ over many lattice distances d between the atoms in a row. This string potential $U(r)$ can be written as

$$U(r) = \frac{1}{d}\int_{-\infty}^{\infty} V[(z^2+r^2)^{\frac{1}{2}}]dz.$$

The integration yields the approximate string potential as

$$U(r) \simeq (z_1 z_2 e^2/d)\ln[(a\sqrt{3}/r)^2+1].$$

This could be approximated into three regions depending upon the projectile energy as follows

$$U_1(r) \simeq 3z_1 z_2 e^2 a^2/r^2 d, \qquad \text{when} \quad r > a\sqrt{3} \tag{1}$$

$$U_2(r) \simeq z_1 z_2 e^2 \pi a/2rd, \qquad \text{when} \quad r \simeq a\sqrt{3}/2 \simeq a \tag{2}$$

and

$$U_3(r) \simeq \frac{z_1 z_2 e^2}{d} \ln\left(\frac{a\sqrt{3}}{r}\right)^2, \qquad \text{when} \quad r < a. \qquad \ldots (3)$$

Though the existing high energy data are in good agreement with eq. (3), some controversies arise in the application of eqs. (1) and (2). Andreen & Hines (1967) measured the angular distribution of keV projectiles of H^+ and $^4He^+$ transmitted through the open channels of thin gold crystals. They found that the observed angular widths in the energy range 2–25 keV studied are in approximate agreement with the expression of critical angle corresponding to eq. (1). Wijngaarden *et al* (1969) found that for channeling of H^+, $^4He^+$, $^{11}B^+$, $^{14}N^+$, $^{20}Ne^+$ and $^{40}Ar^+$ in the open direction of a gold crystal, the energy dependence of the critical angle is closer to an $E^{-1/3}$ dependence, in the energy range 10–60 keV, which corresponds to eq. (2). Bergstorm *et al* (1968) found that for H^+ and $^4He^+$ at energies 20–100 keV, the observed $\psi_{\frac{1}{2}}$ values in the backscattering yield from a tungsten crystal follow much more closely the high energy behaviour than the lower one. Wijngaarden *et al* (1969) have measured the positive charge liberated from a silicon single crystal with ions of appreciably different Z_2 value and in this case also they found a good agreement of their experimental results with eq. (2). Recently, Reuther *et al* (1970) have studied the sputtering and backscattering yields from the (111) surfaces of single crystals of Au, Ag, Al and Si by keV projectiles of H^+ and He^+. They also irradiated Au and Si crystals by various projectiles in the mass range 1–40 a.m.u. It was found that for Si and Au, the channeling behaviour for heavy ions at energies below 100 keV is fairly described by eq. (2). Bhattacharya & Karmohapatro (1973) have measured the backscattering of $^{40}Ar^+$ and $^{20}Ne^+$ from Ag(111) and Ag(100) crystals and their results exhibit an approximate agreement with critical angle expression corresponding to eq. (2). Bhattacharya *et al* (1973) have also measured the sputtering yields of Ag(111) and Ag(100) single crystals with Ar^+, Kr^+ and Xe^+ ions and found an approximate agreement of their results with the theory of Onderdelinden (1968) using expression (2).

To test further, the applicability of the eqs. (1) and (2) in different energy ranges, the scattering angles for gold and silver targets bombarded by argon ions in the energy range 200 eV to 100 keV have been calculated assuming a binary collision model, since it can predict the results within a high accuracy (Mashkova & Molchanov 1972) in the cases considered here. We have used the potentials

$$V(R) = (3/2)Z_1Z_2e^2a^2/R^3, \qquad \ldots (4)$$

and

$$V'(R) = \tfrac{1}{2}Z_1Z_2e^2a/R^2 \qquad \ldots (5)$$

corresponding to eq. (1) and eq. (2) respectively. The results are compared with that of Smith & Carter (1969), who used the Born-Mayer potential for argon ion and a gold atom in the energy range 10 eV to 10 keV.

2. Method

Consider two colliding particles approaching each other with an impact parameter b and a relative kinetic energy E_r as seen from the moving centre of mass of the system. E_r is given by

$$E_r = \frac{AE}{1+A},$$

where E is the true energy in the laboratory frame of reference of the primary moving atom and

$$A = \frac{M_2}{M_1}$$

where M_1 and M_2 are the masses of the projectile and the target atom respectively.

The scattering angle in the centre of mass system θ can be deduced by applying the conservation theorems for energy and angular momentum, which leads to the classical deflection angle formula,

$$\theta = \pi - 2b \int_{R_0}^{\infty} \frac{dR}{R^2\{1-b^2/R^2-V(R)/E_r\}^{\frac{1}{2}}}, \tag{6}$$

where R_0 is the distance of closest approach and is a positive root of the equation

$$1-b^2/R^2-V(R)/E_r = 0. \qquad \ldots \tag{7}$$

Here R is the instantaneous atomic separation and $V(R)$ is the interatomic potential. The true laboratory deflection of scattering angle of the primary moving atom is given by

$$\tan\phi = \frac{A\sin\theta}{1+A\cos\theta}$$

The difficulty arising due to the singular point at the distance of closest approach R_0 in the integrand of eq. (6) is avoided by substituting,

$$\frac{R_0}{1-u^2}$$

as suggested by Robinson (1963). Eq. (6) can now be transformed into a form where the singularity disappears at $u = 0$ as long as

$$\frac{dV(R)}{dR} < 2E_r b^2/R_0^3 \qquad (\text{at } R = R_0)$$

This condition is fulfilled by $V(R)$ and $V'(R)$ represented by eqs. (4) and (5). The transformed integral is evaluated by using 100-step Simpson's rule.

The Ar^+–Au and Ar^+–Ag impact parameters are varied from 0·1 to 1 Å because for larger separations the potential has a value which is too vlarge.

3. Results and Discussion

Figure 1 shows the scattering angle in the laboratory system against impact parameter for Argon ions of 200 eV to 10 keV energies, using $V(R)$ as in eq. (4) for gold target.

Figure 2 shows the same for the same ion-target combination for energies from 5 to 100 keV with $V'(R)$ as in eq. (5).

Figure 3 shows the same for the Ar^+–Ag combination in the energy range as in figure 2 using $V'(R)$ as in eq. (5).

The comparison of our result with that of Smith & Carter (1969) is shown in table 1.

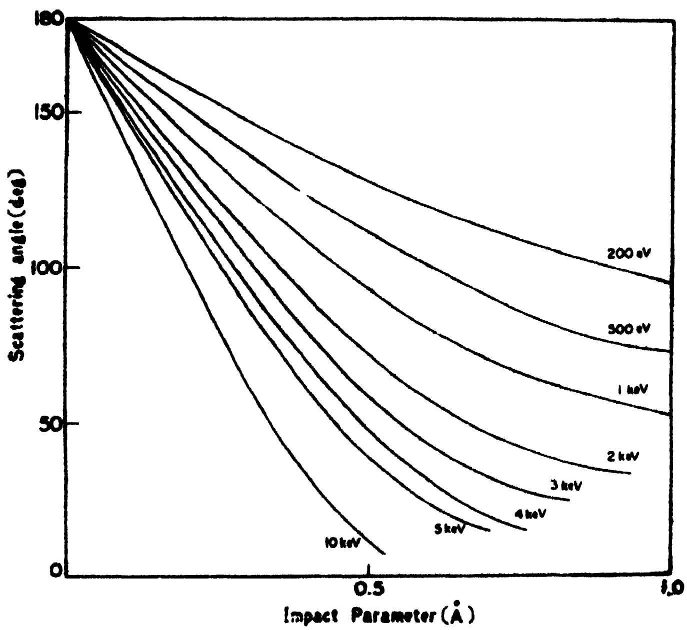

Fig. 1. Scattering angle in the laboratory system against impact parameter for various energies with the interaction potential according to eq. (4) for Ar^+–Au collision.

Table 1 shows that the present data using $V(R)$ as in eq. (4) are closer to those of Smith & Carter (1969) indicating that the potential $V(R)$ as in eq. (4) is suitable for projectile energy for which it is compared. However, it is not possible to suggest which of the Thomas-Fermi or Born-Mayer potentials is more appropriate below the energy 10 keV. Moreover further experiments on back-scattering may be helpful in choosing one of the empirical potentials considered here.

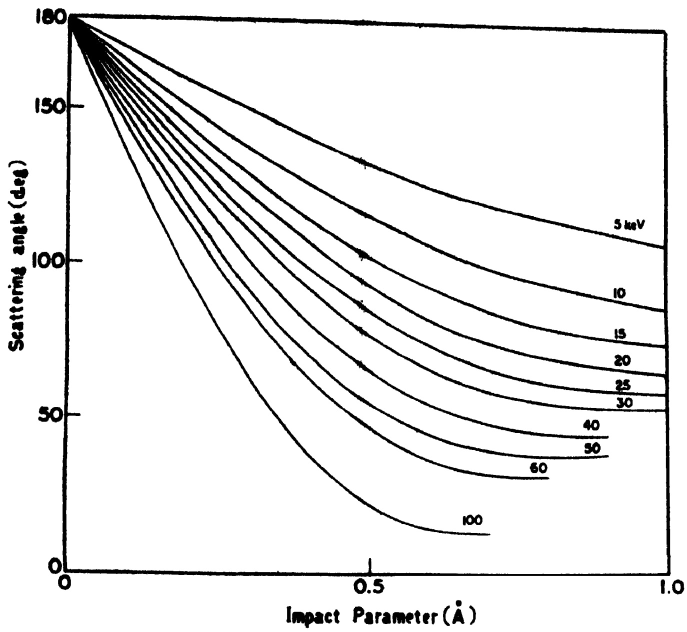

Fig. 2. Scattering angle in the laboratory system against impact parameter for variou energies with the interaction potential according to eq. (5) for Ar^+–Au collision.

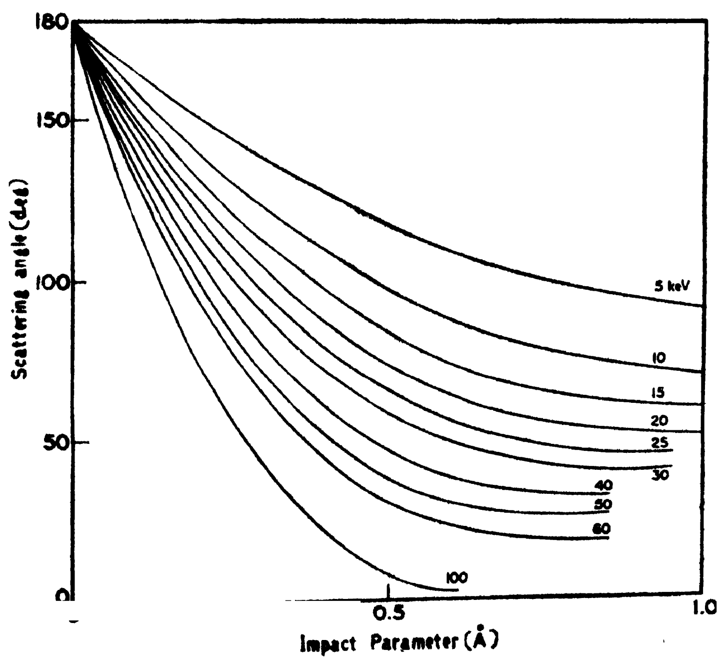

Fig. 3. Scattering angle in the laboratory system against impact parameter for various with the interaction potential according to eq. (5) for Ar^+–Ag collision.

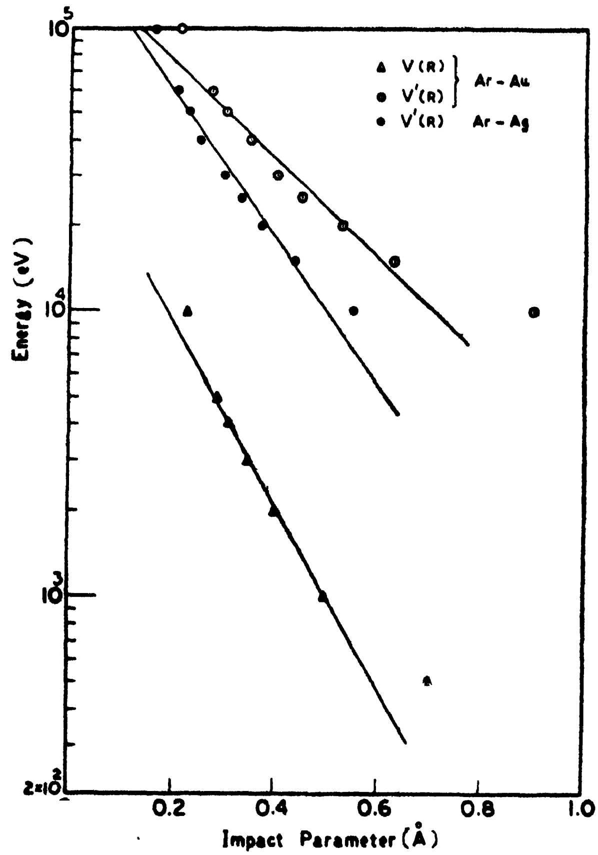

Fig. 4. Energy against impact parameter for a scattering angle of $\pi/2$.

Table 1

Ion energy (in the laboratory system) = 5·0856 keV
Impact parameter = 0·219Å

$R_0 = 0.4960$,	$\sin \frac{1}{2}\theta = 0.8331$	Smith & Carter (1969)
$R_0 = 0.4012$,	$\sin \frac{1}{2}\theta = 0.8829$	Present data (eq. (4))
$R_0 = 1.5083$,	$\sin \frac{1}{2}\theta = 0.9872$	Present data (eq. (5))

Figure 4 deduced from figures 1, 2 and 3 shows the relation between the impact parameter and incident energy at the laboratory scattering angle $\pi/2$, which is important for the backscattering studies. The figure indicates that the applicability of $V(R)$ in the energy range 1–10 keV and $V'(R)$ in 15 to 60 keV approximately is justified in the binary collision model by assuming the logarithmic relation between the impact parameter for $\pi/2$ scattering and the incident ion energy as expected from the analysis by Sigmund & Vajda (1964).

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